Interfacial forces and the fundamental nature of brittle cracks

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A new conception of brittle fracture processes is presented. It is proposed that the crack-tip structure is immutably sharp at the atomic level, such that the attendant growth laws are uniquely determined by the stress intensity factor K of "fracture mechanics" origin. Threshold features in the measured $v(K)$ function for crack growth in interactive environments, previously put forward as evidence for fundamental changes in the tip structure by blunting, are shown to be more consistent with a negative K contribution from interfacial adhesive forces. These adhesive forces should be determinable from the crack velocity characteristics.

The strength of intrinsically brittle materials such as glasses, ceramics, and semiconductors is governed by the growth of small cracks.[1] There would accordingly seem to be good cause to seek an understanding of the "laws" of crack extension at a fundamental level. Nowhere is this cause more apparent than in the rate-dependent fracture properties of brittle materials, where chemically assisted crack growth can lead to premature failures of structural components.[2,3] In this work we shall identify certain aspects of such crack velocity responses which compel us to question the very nature of the brittle fracture process. As a result, we shall make some rather strong new statements concerning the uniqueness of this process in the context of apparent variations in the observed crack velocity laws.

There is a major difficulty which stands in the way of any attempt to model the intrinsic structure of brittle cracks. The stress and strain solutions for a linear elastic continuum slit, upon which all modern-day fracture mechanics is based,[4] are singular at the tip. This singularity does not preclude the definition of a finite "stress intensity factor," K, for quantifying the strength of the crack-tip field: K is readily expressible in terms of externally applied loads and macroscopic crack dimensions and, as such, constitutes a useful parameter for characterizing the crack driving force. However, we *are* precluded from using the solutions to determine the critical crack-tip configurations. The reality is that the material separation processes which operate in this critical region are necessarily nonlinear,[1] reflecting as they must do ultimately the cohesive forces between constituent atoms.

This difficulty has done little to stem the proliferation of crack-tip modeling in the fracture mechanics literature. The development of our thesis requires only that we distinguish between two classes of model, according to whether the crack-tip geometry can be considered "sharp" or "blunt."[5] In the former class, the crack is regarded as retaining the character of a slit, limited in sharpness only by the atomic bonds which hold the opposing walls together at the tip.[6–9] In the latter class, a certain continuum-scale roundness is ascribed to the tip region.[10] The usefulness of this distinction lies in the fact that for given driving forces on the crack system the tip configurations, and hence the appropriate crack velocity relations $v(K)$, are uniquely determined in just the first class; with the blunt-crack representations tip radius enters as a controlling geometrical factor, thereby introducing a structure-extrinsic, history-dependent element into the velocity relations.[5]

Those who suport the rounded-crack hypothesis point to two key fracture studies on glass in water environment. Mould[11] showed that the strength of specimens containing abrasion microcracks increases with aging time (i.e., time between abrasion and testing to failure). Michalske[12] noted that the velocity function $v(K)$ exhibits a low K threshold. The consensus from these studies was that the results could only be explained in terms of retardation in crack growth by blunting.

A recent study conducted in these laboratories suggests that this consensus is ill founded.[5] Our experiments originally set out to duplicate the aging tests of Mould, but using indentation rather than abrasion microcracks. The critical advantage here was that, by viewing the glass specimens in polarized light, the evolution of the indentation cracks could be followed directly throughout the aging period. It was thereby observed that the cracks actually extend during the aging. At the same time, residual tensile stresses associated with the irreversible component of the contact deformation showed a progressive diminution. The unequivocal conclusion was that it is the relaxation in pre-existing crack driving forces and not a change in the crack-tip geometry which is responsible for Mould's strengthening effect.

However, the implications of the indentation experiments were more far reaching.[5] The *rate* of crack extension fell off rapidly with time of aging until ultimately, at about 75% residual stress relaxation, it dropped to zero. It could be shown that the crack system had progressed down the $v(K)$ curve to the threshold K level. At this point (attained after ≈ 1 day) and thereafter (for aging periods up to 3 months) the strengthening saturated out. But it is precisely in the threshold region where blunting is supposed to be operating,[12] in which case we should expect a dramatic rise, not a saturation, in strength. The argument seemed compelling that if the cracks remain sharp during the first stage of aging (i.e., when the strength *did* show an increase) they must also remain sharp on the long-term plateau. The fact that similar strength plateaus are observed in far more corrosive aging environments, e.g., *boiling* water[13] or even HF acid solutions,[5] suggests that this intrinsic sharpness is not easily negated under any conditions.

We are now left with the vital question: If blunting is excluded as a mode of crack retardation, then what *is* the cause of the $v(K)$ threshold? We propose a mechanism involving interfacial adhesive forces. In highly brittle materials the crack wall separation remains extremely narrow for

some distance behind the tip,[7] particularly at the relatively low threshold K levels. We view the interface as something akin to a grain boundary (albeit dilated), where intruding chemical species are constrained to assume a two-dimensional ordered structure as they approach the critical crack-tip bonds.[14] It is not difficult to see how substantial adhesive forces might arise with such a configuration. None of this is to imply that the crack tip is immune to environmental attack. Rather, the chemical processes which operate *at* the crack tip, by virtue of a strong tendency to specificity associated with the highly localized state of strain there, are seen to operate independently of those processes which might occur *behind* the tip. In this picture interfacial forces play no part in determining the fundamental $v(K)$ function, yet may exert a significant influence on the fracture kinetics by contributing to the net driving force K on the crack.

Our proposal is not without experimental justification. The most direct confirmation comes from crack healing experiments in which the fracture system is subjected to a closing and reopening cycle. Tests on mica[15] and glass[16,17] in moist environments show that a nonzero applied force is necessary to repropagate the crack through the closed interface, although this force is usually much less than that needed to drive the original crack. In another set of experiments, Israelachvili and co-workers,[18,19] using a delicate microbalance, have been able to measure forces between opposing surfaces of mica down to atomic-scale separations. Again, colloid chemists are able to make particulate suspensions coagulate (or disperse) by manipulating the solution pH.[20] The energies of adhesion vary considerably depending on the interfacial species, but can exceed 100 mJ m^{-2}, i.e., typical of weak, long-ranged interactions. The question is, are these energies large enough to account for the observed crack velocity behavior, particularly in the threshold region?

To place our hypothesis on a quantitative footing we consider the fracture mechanics model in Fig. 1. A straight-fronted crack of length c and thickness unity is subjected to externally applied loading which generates a driving force, K_a, at the tip. Attractive interfacial stresses $\sigma_i(x)$ active over a small distance d behind the tip generate a second driving force, K_i. This second contribution can be formulated in the manner of Barenblatt's "modulus of cohesion," in the limit $d \ll c$,[6]

$$K_i = -\left(\frac{2}{\pi}\right)^{1/2} \int_0^d x^{-1/2}\, \sigma_i(x) dx. \tag{1}$$

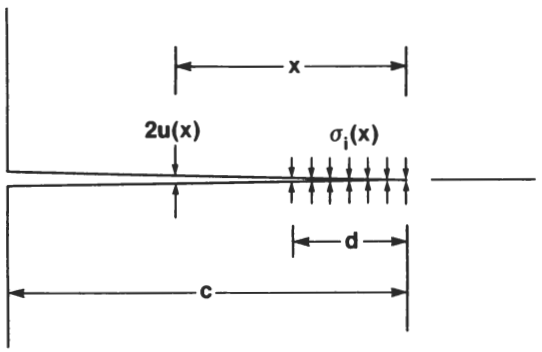

FIG. 1. Interfacial adhesive force model of crack retardation.

Clearly, explicit evaluation of Eq. (1) requires *a priori* knowledge of $\sigma_i(x)$, which is not generally available. A simplifying approximation here is to neglect the disturbance of the interface stresses on the geometry (but not the intensity) of the local displacement field, so that the standard crack-profile solution may be retained for the crack in combined loading, $K = K_a + K_i$; (Ref. 4) i.e.

$$u(x) = (K/E)(8x/\pi)^{1/2}, \tag{2}$$

where E is Young's modulus. Now x may be eliminated from Eqs. (1) and (2) to give

$$\begin{aligned} K_i &= -\left(\frac{E}{K}\right) \int_0^{u(d)} \sigma_i(u) du \\ &= -E\gamma_i/K, \end{aligned} \tag{3}$$

where $2\gamma_i$ defines the work to separate the crack walls to the stress-free state. Note the inverse relationship between K_i and K; on reducing the net crack driving force the opposing crack walls come closer together, bringing a greater area of interface within the "range" $u(d)$ of adhesion.

The above analysis allows us to determine a useful connecting relation between K and K_a. We may use Eq. (3) to write the net crack-tip driving force as

$$K = K_a - E\gamma_i/K. \tag{4}$$

Plots of the function $K(K_a)$ are shown in Fig. 2, for $\gamma_i = 0, > 0$, and < 0. The case $\gamma_i = 0$ is trivial, giving the zero-interaction line $K = K_a$. For $\gamma_i \neq 0$, the interfacial term effectively screens the tip from the remote loading, giving rise to a systematically increasing departure from the $K = K_a$ line at low K values. The curve for $\gamma_i > 0$ (attractive forces) bends down to a threshold, $K_a = K_{th}$, at

$$K_{th} = 2(E\gamma_i)^{1/2} \tag{5}$$

below which the crack closes and heals spontaneously. The curve for $\gamma_i < 0$ (repulsive forces) bends upwards, but always remains a monotonically decreasing function with diminishing K_a.

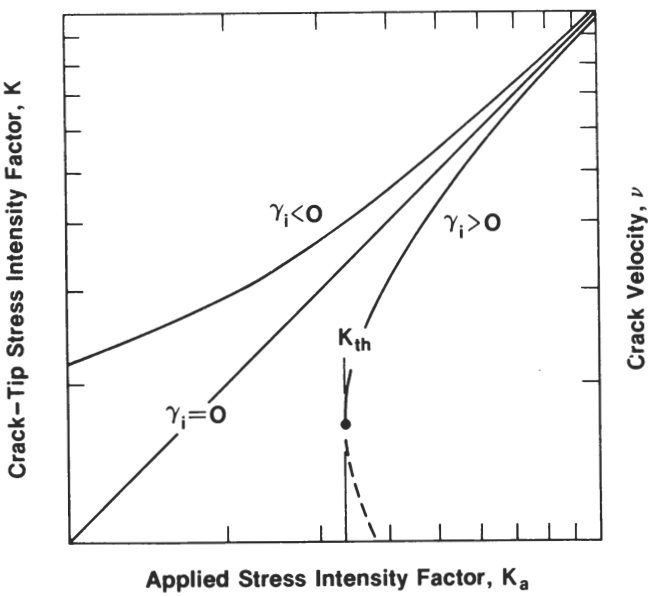

FIG. 2. Plots of $K(K_a)$, or equivalently $v(K_a)$, for γ_i zero, positive and negative. (Axes plotted in logarithmic coordinates, consistent with commonly adopted power law v-K relation for brittle materials.)

The link between this formulation and the crack velocity function is straightforward. We reassert that the crack-tip configuration remains invariably sharp and so is uniquely determined by the net K. This configuration in turn uniquely determines the rate of extension for given environmental conditions. Hence the vertical axis in Fig. 2 may equivalently be regarded as a velocity axis (the scaling, of course, depending on the intrinsic $v(K)$ relation). Thus we should expect the curves in Fig. 2 to be indicative of the $v(K_a)$ relation one would measure by monitoring the applied load in an actual crack velocity experiment.

Let us compare predictions from our analysis with experimental data on the crack velocity threshold for soda-lime glass in water. Michalske[12] cites 0.25 MPa $m^{1/2}$ for K_{th} from earlier data by Wiederhorn and Bolz.[21] Taking $E = 70$ GPa for glass[21] and $\gamma_i = 100$ mJ m^{-2}, Eq. (5) gives 0.17 MPa $m^{1/2}$. Allowing that we have used only a "typical" value of γ_i here, and that our theory is only approximate, we see that we have the capacity to account quantitatively for threshold effects without recourse to blunting.

There are other features in the observed velocity data for glasses which are consistent with our model. It is well known that the $v(K_a)$ curves for a given glass may shift with changes in environmental conditions (especially solution pH), or indeed for a given environment with changes in glass composition.[22] As we see from Fig. 2, such shifts may result (at least in part) as a natural consequence of the strong sensitivity of γ_i to chemical conditions alluded to earlier. Special mention may be made of the fact that the observed shifts include those in the direction of the upper curve in Fig. 2,[23] i.e., consistent with repulsive interactions. It is difficult to see how a tendency to an *enhancement* in velocity can be reconciled with any blunting hypothesis.

The decoupling of events at the crack interface from those at the tip has interesting scientific implications. On the one hand, it establishes the brittle crack as a stress-specific, molecular-intrinsic entity worthy of fundamental study. This should provide some impetus to those who seek to describe crack-tip structure at the atomic level, e.g., in terms of lattice models,[24,25] molecular orbitals,[26] etc. On the other, it offers the prospect to surface and colloid chemists of a new technique for measuring surface forces, via the $v(K_a)$ response. Here the difficulty which has restricted most previous force measurements to one material (mica), i.e., that of obtaining atomically smooth contacts, is overcome by the very nature of the geometrical constraints which exist just behind the crack tip.

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